density map using the MDFF method (Molecular Dynamics Flexible Fitting). The structure allowed for the identification of ribosome–lipid interactions. The rRNA helix 59 (H59) directly contacts the lipid surface and appears to modulate the membrane in immediate vicinity to the proposed lateral gate of the PCC. Based on our map and molecular dynamics simulations we present a model of a signal anchor–gated PCC in the membrane.

**Keywords: cryo-EM, SecYEG, MDFF,**

## MS.02.2

*Acta Cryst.* (2011) A**67,** C25

**Dynamics and stability in virus maturation: mechanisms of a molecular machine**

John E. Johnson, *Department of Molecular Biology The Scripps Research Institute La Jolla, C A, (USA).*

Assembly of quasi-equivalent virus capsids engages molecular switches to create different interface contacts between the same gene products. The particle often assembles as a fragile, spherical shell in which the subunits are properly positioned on the appropriate surface lattice and then quasi-equivalent subunit contacts differentiate during maturation, creating a robust, faceted particle. Folding of the switch regions of the subunit depends on assembly and maturation that are affected by biochemical cues. NwV is a quasi-equivalent virus, with a *T*=4 surface lattice, where this process is dramatic (a change in particle size of 100Å during maturation) and can be investigated *in vitro*. Here we use biochemistry [1], Small Angle X-ray Scattering [2] and electron cryo-microscopy and image reconstruction (CryoEM) [3] to characterize maturation intermediates and an associated auto-catalytic cleavage, the kinetics of morphological change and to demonstrate that regions of NwV subunit folding are maturation-dependent and occur at rates determined by their quasi-equivalent position in the capsid.

[1] T. Matsui, G. Lander, J.E. Johnson, *J Virol* **2009,** *83,* 1126-1134. [2] T. Matsui, G. Lander, R. Khayat, J.E. Johnson, *Proc. Natl. Acad. Sci. USA,* **2010,** *107,* 14111-5. [3] T. Matsui, H. Tsuruta, J.E. Johnson, *Biophys J.* **2010,** *98*, 1337-43.

**Keywords: virus, dynamics, maturation**

## MS.02.3

*Acta Cryst.* (2011) A**67,** C25

**Lessons learned from the cryoEM and x-ray structures of the human adenovirus**

Z. Hong Zhou,[a,b] Hongrong Liu,[a,b,c] [a] *Department of Microbiology, Immunology & Molecular Genetics, University of California, Los Angeles (UCLA) (USA).* [b]*California NanoSystems Institute, UCLA, Los Angeles, CA 90095 (USA).* [c]*Institute of Modern physics, Xiangtan University, Xiangtan, Hunan 411105 (China).* E-mail: Hong.Zhou@UCLA.edu

Structural information of macromolecular complexes in the form of atomic coordinates is essential to uncovering the mechanisms of action of biological functions and to designing compounds for therapeutic interventions of human diseases. X-ray diffraction and Nuclear magnetic resonance spectroscopy (NMR) have been very successful in solving atomic structures of biomedical importance and are the primary contributors of atomic structures determined to date. The emerging technology of single-particle cryo electron microscopy (cryoEM) has less stringent requirement for sample purity and quantity than x-ray crystallography and NMR but resolution achieved by cryoEM is often limited to nanometer or molecular resolutions, thus severely limited its value and application in biomedical research.

Recently, several cryoEM structures have crossed the resolution barrier of 4 Å. This progress in cryoEM was made possible by a number of advancements, such as atomic-resolution image acquisition and efficient molecular model building. Of special note, the structure of the human adenovirus has been determined by both methods of cryo-EM and x-ray crystallography, independently by two groups. Here we provide the first direct comparisons (Figure 1) of these cryoEM [1] and x-ray structures [2], at resolutions of 3.6 Å and 3.5 Å, respectively. This comparison shows an excellent match between the structures of the "major" proteins, revealed by the cryoEM and x-ray structures of the human adenovirus. It also highlights significantly richer information content in the cryoEM structures of the three "minor" proteins IIIa, VIII and IX, which play essential role in adenovirus assembly and genome packaging. In particular, extended regions in these proteins that are involved in molecular interactions are resolved in the cryoEM structure, but not in the x-ray structure. These results support our argument that cryoEM offers advantages over x-ray crystallography in studying the structure of large macromolecular complexes with flexible and transiently stable structural elements [3].

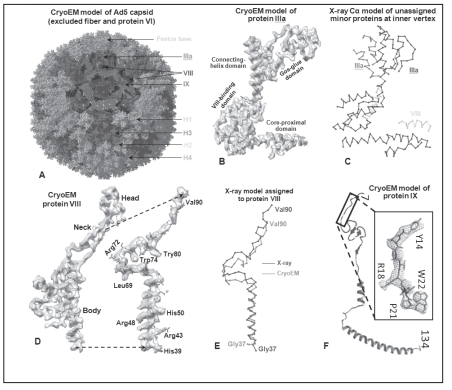


**Figure 1. Comparison of cryoEM and XDR structure of the human adenovirus.** (A) CryoEM atomic model. (B-C) Minor protein IIIa. (D-E) Minor protein VIII. (F) CryoEM model of protein IX.

[1] H. Liu, L. Jin, S.B. Koh, I. Atanasov, S. Schein, L. Wu, Z.H. Zhou. *Science* **2010,** *329,* 1038-1043. [2] V.S. Reddy, S.K. Natchiar, P.L. Stewart, G.R. Nemerow, *Science* **2010,** *329,* 1071-1075. [3] Supported in part by NIH grants GM071940 and AI069015.

**Keywords: adenovirus, cryoEM, x-ray crystallography**

## MS.02.4

*Acta Cryst.* (2011) A**67,** C25-C26

**Crystal structure of the open conformation of the mammalian chaperonin CCT in complex with tubulin**

Inés G. Muñoz,[a] Hugo Yébenes,[b] Min Zhou,[c] Pablo Mesa,[b] Marina Serna,[b] Ah Y. Park,[c] Elisabeth Bragado-Nilsson,[a] Ana Beloso,[b] Guillermo de Cárcer,[d] Marcos Malumbres,[d] Carol V. Robinson,[c] José M. Valpuesta,[b] Guillermo Montoya,[a] [a]*Macromolecular Crystallography Group, Structural Biology and Biocomputing Programme, Spanish National Cancer Research Centre (CNIO), Madrid, (Spain).* [b]*Centro Nacional de Biotecnología, CSIC, Campus de la Universidad Autónoma de Madrid, Madrid, (Spain).* [c]*Department of Chemistry, Physical and Theoretical Chemistry Laboratory, Oxford, (UK).* [d]*Cell Division & Cancer Group, Molecular Oncology Programme, Spanish National Cancer Research Centre (CNIO), Madrid, (Spain).* E-mail: imunoz@cnio.es

Protein folding is assisted by molecular chaperones. CCT